数理解析研究所講究録
905巻 1995年 6-14

A NOTE ON THE EXISTENCE OF UNITARY PROPAGATOR OF EQUATIONS IN QUANTUM MECHANICS

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1. Introduction.

In this talk we study the equation

$$(*)\quad i\hbar\frac{\partial u}{\partial t}(t) = K(t)u(t)\ (0 \le t \le T), u(0) = f \in (L^2)^N$$

$$(u(t) = {}^t(u_1(t), \dots, u_N(t)))$$

describing the motion of some charged particles in an electromagnetic field $E(t), B(t)$, where i is the imaginary unit, $\hbar$ the Planck constant over 2π, and $(L^2)^N$ the product space of N copies of the space of all square integrable functions. The norm $\|f\|$ of $f \in (L^2)^N$ is defined by $(\sum_{j=1}^N \int |f_j(x)|^2 dx)^{1/2}$.

We are concerned with the existence and uniqueness of unitary propagator $U(t)$, i.e. $U(t)f$ belongs to $\mathcal{E}_t^0([0,T];(L^2)^N)$ and is the solution of $(*)$ such that $\|U(t)f\| = \|f\|$ $(0 \le t \le T)$. We denote by $\mathcal{E}_t^j([0,T];F)$ the space of all F-valued j times continuously differentiable functions in $[0,T]$.

Suppose that $K(t)$ is independent of t. That is, suppose that $E(t)$ and $B(t)$ are independent of t. Then it follows from Stone's Theorem that the existence and uniqueness of $U(t)$ is virtually equivalent to the self-adjontness of K on $(L^2)^N$. The self-adjointness or the essential self-adjointness of K has been studied in much detail. So in this talk we consider the case that $E(t)$ and $B(t)$ vary in time t.

The results and their complete proofs in this talk will be published in Osaka J. Math.

2. Typical equations.

Let $x \in R^n$, $V(t,x)$ the scalar potential, and $A(t,x) = (A_1, \cdots, A_n)$ the vector potential. Typical equations we consider are as follows.

(1) Schrödinger's equation. $N = 1$.

$$K(t)g = \{\frac{1}{2}\sum_{j=1}^{n}(\hbar D_{x_j} - A_j)^2 + V\}g \quad (D_{x_j} = \frac{1}{i}\frac{\partial}{\partial x_j}).$$

(2)Pauli's equation. $n = 3$.

$$K(t)g = \{\frac{1}{2}\sum_{j=1}^{3}(\hbar D_{x_j} - A_j)^2 + V\}g - \frac{\hbar}{2}\sum_{j=1}^{3} B_j(t,x)\sigma_j g,$$

where σ_j $(j = 1, \cdots, n)$ are N by N Hermitian matrices.

(3) Dirac's equation.

$$K(t)g = \{c\sum_{j=1}^{n}\alpha_j(\hbar D_{x_j} - A_j) + \beta c^2 + V\}g,$$

where α_j and β are N by N Hermitian matrices. $c > 0$ is the velocity of light.

(4) The equation of a relativistic spinless particle. $N = 1$.

$$K(t)g = k(t, \frac{X + X'}{2}, \hbar D_x)g \quad \text{(Weyl's operator)}$$
$$:= (2\pi)^{-n} \iint e^{i(x-x')\cdot\xi} k(t, \frac{x + x'}{2}, \hbar\xi) g(x') dx' d\xi,$$

where $k(t, x, \xi) = c\sqrt{c^2 + |\xi - A|^2} + V$.

3. Results.

We assume that $V(t, x)$ and $A(t, x)$ are smooth in x. We first introduce one of Yajima's results in J. D'Analyse Math., '91. See also Fujiwara, J. D'Analyse Math., '79, Kitada, J. Fac. Sci. Univ. Tokyo Sec. IA, '80, and Robert, Birkhäuser, '87.

By using the Gauge transformation we may suppose

$$V(t, x) = 0.$$

Set

$$B_{jk}(t, x) = \frac{\partial A_k}{\partial x_j}(t, x) - \frac{\partial A_j}{\partial x_k}(t, x).$$

Assume the following. There exists a positive constant δ such that

$$\sum_{j,k=1}^{n} |\partial_x^\alpha B_{jk}(t, x)| \le C_\alpha < x >^{-(1+\delta)} \text{ for all } \alpha \neq 0,$$
$$\sum_{j=1}^{n} \{|\partial_x^\alpha A_j(t, x)| + |\partial_t \partial_x^\alpha A_j(t, x)|\} \le C_\alpha \text{ for all } \alpha \neq 0,$$

where $< x >= \sqrt{1 + |x|^2}$. Then, he constructed the fundamental solution of Schrödinger's equation by using the Fourier integral operator. From this we can prove the existence and uniqueness of $U(t)$.

Remark. Yajima's main purpose is to show the existence and uniqueness of $U(t)$ of Schrödinger's equation with potentials having singularities, like that $V = -1/|x - g(t)|$. □

We note that Yajima's result is not general. For example, his result doesn't include the case $A_j(t,x)$ is periodic in x. We report in this talk :

(1) We can extend Yajima's result on Schrödinger's equation. For example, we can see the existence and uniqueness of $U(t)$ in the case $A_j(t,x)$ is periodic in x.

(2) We can get the similar result on the other equations (Pauli's, Dirac's, and the equation of a relativistic spinless particle).

Theorem 1. Let $(k_{jl}(t,x,\xi))_{j,l=1}^N$ be an N by N Hermitian matrix such that the assumption (A) or (B) below is satisfied. Set $K(t) = (k_{jl}(t, \frac{X+X'}{2}, \hbar D_x))_{j,l=1}^N$. Then, we can see the existence and uniqueness of the unitary propagator $U(t)$ of $(*)$.

(A) We have for all $\alpha + \beta \neq 0$

$$\sum_{j,l=1} |k_{jl(\beta)}^{(\alpha)}(t,x,\xi)| \leq C_{\alpha,\beta}(1 + |x| + |\xi|),$$

where $k_{jl(\beta)}^{(\alpha)}(t,x,\xi) \ = \partial_\xi^\alpha D_x^\beta k_{jl}(t,x,\xi)$.

(B) (i) We have for all $\alpha \neq 0$ and β

$$\sum_{j,l=1} |k^{(\alpha)}_{jl(\beta)}(t,x,\xi)| \leq C_{\alpha,\beta}.$$

(ii) There exists a constant $M \geq 1$ such that for all β

$$\sum_{j,l=1} |k_{jl(\beta)}(t,x,\xi)| \leq C_\beta(< x >^M + < \xi >). \quad \Box$$

Application to Schrödinger's and Pauli's equation. Assume that $\sum_{j=1}^n |\partial_x^\alpha A_j| \leq C_\alpha$ for all $\alpha \neq 0$ and $|\partial_x^\alpha V| \leq C_\alpha < x >$ for all $\alpha \neq 0$. Then we can see the existence and uniqueness of $U(t)$. $\Box$

Application to Dirac's equation. Assume the following. There exists a constant $M \geq 1$ such that $\sum_{j=1}^n |\partial_x^\alpha A_j(t,x)| + |\partial_x^\alpha V(t,x)| \leq C_\alpha < x >^M$ for all α. Then we can see the existence and uniqueness of $U(t)$. $\Box$

Application to the equation of a relativistic spinless particle. Assume the following. We have $\sum_{j=1}^n |\partial_x^\alpha A_j| \leq C_\alpha \log < x >$ for all $\alpha \neq 0$ and there exists a constant $M \geq 1$ such that $|\partial_x^\alpha V(t,x)| \leq C_\alpha < x >^M$ for all α. Then we can see the existence and uniqueness of $U(t)$. $\Box$

Let $s \geq 0$ and define weighted Sobolev's spaces $B^s_{a,b}(\hbar)$ by $\{f \in L^2; \|f\|_{B^s_{a,b}(\hbar)} \equiv \| < \cdot >^{as} f\| + \| < \hbar \cdot >^{bs} \hat{f}\| < \infty\}$ $(a \geq 0, b \geq 0)$. We denote its dual space by $B^{-s}_{a,b}(\hbar)$. Then we can get a more detailed result than Theorem 1.

Theorem 2. (i) Assume (A). Let $f \in B^s_{1,1}(\hbar)^N$ $(s \geq 0)$. Then the solution $U(t)f$ of $(*)$ belongs to $\mathcal{E}^0_t([0,T]; B^s_{1,1}(\hbar)^N) \cap \mathcal{E}^1_t([0,T]; B^{s-2}_{1,1}(\hbar)^N)$. In addition, there exists a constant $C_s(T)$ independent of $0 < \hbar \leq 1$ such that

$$\|U(t)f\|_{B^s_{1,1}(\hbar)^N} \leq C_s(T)\|f\|_{B^s_{1,1}(\hbar)^N} \quad (0 \leq t \leq T).$$

(ii) Assume (B). Let $f \in B^s_{M,1}(\hbar)^N$. Then the solution $U(t)f$ belongs to $\mathcal{E}^0_t([0,T]; B^s_{M,1}(\hbar)^N) \cap \mathcal{E}^1_t([0,T]; B^{s-1}_{M,1}(\hbar)^N)$, where M is the constant appearing in (B). In addition, we get the same inequality as in (i) where $B^s_{1,1}(\hbar)$ is replaced by $B^s_{M,1}(\hbar)$. □

The above inequalities are important in the study of the classical limit (c.f. Wang, Commun. Math. Phys., '86).

4. The outline of the proof of Theorems. We first give the outline of the proof of Theorem 1. Let $N = 1$. The general case can be proved similarly. We define $\omega(x,\xi)$ by

$$\omega(x,\xi) = \begin{cases} <x> + <\xi>, & \text{when (A) is assumed,} \\ <x>^M + <\xi>, & \text{when (B) is done.} \end{cases}$$

We give the proof under (A). That under (B) is similar.

Let $\chi(\theta)$ be a real valued and infinitely differentiable function on R^1 with compact support such that $\chi(0) = 1$. Let $0 < \epsilon \leq 1$ and set

$$k_\epsilon(t,x,\xi) = \chi(\epsilon\omega(x,\xi))k(t,x,\xi).$$

We note that $\lim_{\epsilon \to 0} k_\epsilon(t,x,\xi) = k(t,x,\xi)$ pointwisely.

We first consider

$$(*)_\epsilon \quad i\hbar\frac{\partial u}{\partial t}(t) = K_\epsilon(t)u(t) \equiv k_\epsilon(t, \frac{X+X'}{2}, \hbar D_x)u(t),$$
$$u(0) = f$$

in place of $(*)$.

1st step. Assume $f \in B^2(\hbar) := B^2_{1,1}(\hbar)$. Note that $k_\epsilon(t,x,\xi)$ is a infinitely differentiable function on $R^{2n}_{x,\xi}$ with compact support. So we can easily show that $K_\epsilon(t)$ is a bounded operator on $B^2(\hbar)$. Consequently we can prove by using the iteration that there exists a solution $u_\epsilon(t) \in \mathcal{E}^1_t([0,T]; B^2(\hbar))$ of $(*)_\epsilon$. Then we can easily have

$$\|u_\epsilon(t)\| = \|f\|.$$

Now using the assumption (A), we can prove that

$$\{u_\epsilon(t)\}_{0<\epsilon\leq 1} \text{ is a bounded family in } \mathcal{E}^0_t([0,T]; B^2(\hbar))$$

and that

$$\{K_\epsilon(t)\}_{0<\epsilon\leq 1} \text{ is a bounded one in the space of operators from } B^2(\hbar) \text{ into } L^2.$$

These are essential in our proof. We omit their proofs.

Since

$$i\hbar u_\epsilon(t) - i\hbar u_\epsilon(t') = \int_{t'}^t K_\epsilon(s)u_\epsilon(s)ds,$$

we see from the results above that

$$\{u_\epsilon(t)\}_{0<\epsilon\le 1} \text{ is an equi-continuous family in } \mathcal{E}_t^0([0,T];L^2).$$

We note that the embedding map from $B^2(\hbar)$ into L^2 is compact. Hence we can apply Ascoli-Arzelà's theorem to a family $\{u_\epsilon(t)\}_{0<\epsilon\le 1}$ in $\mathcal{E}_t^0([0,T];L^2)$. So there exist a function $u(t)$ and a sequence $\epsilon_1 > \epsilon_2 > \cdots \to 0$ such that

$$u_{\epsilon_j}(t) \to u(t) \quad \text{in} \quad \mathcal{E}_t^0([0,T];L^2).$$

We can prove that this $u(t)$ belongs to $\mathcal{E}_t^1([0,T];B^{-2}(\hbar))$ and satisfies $(*)$. Thus, we could find a solution $u(t) \in \mathcal{E}_t^0([0,T];L^2) \cap \mathcal{E}_t^1([0,T];B^{-2}(\hbar))$ such that $\|u(t)\| = \|f\|$.

2nd step. In this step we will show the uniqueness of the solution of $(*)$. Let $g(t) \in B^4(\hbar)$ and consider the equation

$$i\hbar\frac{\partial v}{\partial t}(t) = K(t)v(t) + g(t) \ (0 \le t \le T), \ v(T) = 0.$$

As in the proof in the 1st step we get a solution $v(t) \in \mathcal{E}_t^0([0,T];B^2(\hbar)) \cap \mathcal{E}_t^1([0,T];L^2)$.

Let $u(t) \in \mathcal{E}_t^0([0,T];L^2)$ be a solution of $(*)$ with $u(0) = 0$. Then $u(t) \in \mathcal{E}_t^1([0,T];B^{-2}(\hbar))$ follows from $(*)$. So we have

$$0 = \int_0^T (i\hbar\frac{\partial u}{\partial t}(t) - K(t)u(t), v(t))dt = \int_0^T (u(t), g(t))dt.$$

Hence we have $u(t) = 0$, because $g(t)$ is arbitrary. $\square$

3rd step. Let $f \in L^2$. Then there exists a sequence $f_j \in B^2(\hbar)$ $(j = 1, 2, \cdots)$ such that $f_j \to f$ in L^2. It follows from the 1st and 2nd steps that a solution $u_j(t) \in \mathcal{E}_t^0([0,T]; L^2) \cap \mathcal{E}_t^1([0,T]; B^{-2}(\hbar))$ of $(*)$ to f_j is determined uniquely and we have

$$\|u_j(t)\| = \|f\|.$$

In addition, since $u_j(t) - u_k(t)$ is the solution of $(*)$ to $f_j - f_k$ determined uniquely, we also have

$$\|u_j(t) - u_k(t)\| = \|f_j - f_k\|.$$

Consequently there exists a $u(t) \in \mathcal{E}_t^0([0,T]; L^2)$ such that

$$u_j(t) \to u(t) \text{ in } \mathcal{E}_t^0([0,T]; L^2).$$

We can prove that this $u(t)$ belongs to $\mathcal{E}_t^1([0,T]; B^{-2}(\hbar))$ and is a solution of $(*)$ satisfying $\|u(t)\| = \|f\|$. The uniqueness of the solution has already been proved in 2nd step. Thus the proof of Theorem 1 could be completed.

We can prove Theorem 2 by the analogous arguments used in the proof of Theorem 1. $\square$